

Workshop Report Schedule

Large Scale Computing and Storage Requirements for Basic Energy Sciences Research

Joint BES / ASCR / NERSC Workshop

February 9-10, 2010









Logistics: Final Report Content

- Overview
 - Executive Summary (NERSC writes)
 - Findings (NERSC)
 - NERSC Response
- BES Goals (DOE writes)
- Chemistry, Materials, Geosciences goals
- Case studies: specific examples
 - What scientific questions will be addressed
 - What's needed from NERSC to do so







Logistics: Final Report Content

- Key element of case studies: how science goals drive NERSC requirements
 - Want a direct relationship between specific science goals and NERSC needs
 - "In 3 years we want to be able to study 'X' but to do so requires '1,2,3' "
 - Or "Having access to 50x resources will allow us to resolve 'X' or understand 'Y' "
 - Etc.







Input

- Basically 3 inputs
 - The worksheet you filled out already;
 - The case study template and examples from previous NERSC BER workshop;
 - Other considerations that came up during discussions on Tuesday and Wednesday
 - Either full-group or during science area telecons







Logistics: Final Report Schedule

- Case studies due to NERSC: March 8
- NERSC draft report: April 2
- Participants review period: April 2-16
- NERSC Near final: April 30
- BER AD approval: May 7
- NERSC Revisions: May 21
- Final Report posted: June 4

Important participant deadlines in red







Examples of Information Sought

- Type of simulation, #, reason for #, algorithms, solver
- Parallelism: method, weak or strong scaling, implementation, concurrency, limits
- Key physical parameters and their limits:
 - spatial resolution, # of atoms/energy levels, integration range, ...
- Representative code
- Key science result metrics and goals







Examples of Information Sought

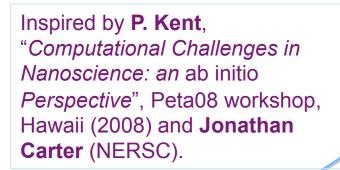
- Typical science process (workflow)
- Data: amount stored / transferred for input, results, and fault mitigation
- Special needs for data intensive projects
 - Grids, gateways, workflows, provenance, `
- Special query regarding multicore/manycore
- How all of this is
 - Driven by the science
 - Likely to change and why







Scaling Science



Length, Spatial extent, #Atoms, Weak scaling

Convergence, systematic errors due to cutoffs, etc.

Time scale Optimizations, *Strong scaling*

Initial Conditions, e.g. molecule, boundaries,

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Simulation method, e.g. DFT, QMC or HF/ SCF; LES or DNS